

Molecular Pairing and Fully-Gapped Superconductivity in Yb doped CeCoIn₅

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Abstract

The recent observation of fully-gapped superconductivity in Yb doped CeCoIn₅ poses a paradox. Naively, the disappearance of nodes suggests that they are accidental, however nodal d-wave symmetry is well established in this material by scanning tunneling spectroscopy and angle resolved thermal conductivity measurements. Here we suggest that composite pairing can provide a natural resolution to the paradox. We propose that Yb doping changes the chemical potential, driving a Lifshitz transition that depletes the Fermi surface, giving rise to a fully-gapped “Kondo insulator” immersed within a d-wave molecular condensate. In this fully-gapped phase, the temperature dependence of the penetration depth is proportional to $\Delta\lambda(T) \sim T^3$ for temperatures greater than the plasma frequency in accord with observations. We conclude with various predictions for future experiments.

Introduction: CeCoIn₅ is an archetypal heavy fermion superconductor with $T_c = 2.3K$ [1]. The Curie-Weiss susceptibility signaling unquenched local moments, persists down to the superconducting transition [1]. Local moments, usually harmful to superconductivity actually participate in the condensate and a significant fraction of the local moment entropy ($0.2 - 0.3 \log 2$ per spin) is quenched at T_c .

The behavior of this material becomes even more surprising upon Yb doping. Firstly, superconductivity is extremely stable and the transition temperature has the unusual form $T_c(x) = T_c(0) \times (1 - x)$, where x is the Yb doping[2]. Moreover recent experiments[3] on the temperature dependence of the London penetration depth $\Delta\lambda(T)$ show that nodal d-wave superconductivity (where $\Delta\lambda(T) \sim T - T^2$), becomes fully gapped ($\Delta\lambda(T) \sim T^n, n \sim 3$) after a critical Yb doping ($x \sim 0.2$). Normally the disappearance of nodes would suggest that they are accidental as in s^\pm superconductors. However directional probes of the gap, including scanning tunneling spectroscopy (STM)[4], thermal conductivity measurements in a rotating magnetic field[5] and torque magnetometry[6] strongly suggest it is a nodal d-wave superconductor. This raises the question: *How can nodal d-wave superconductor become fully-gapped upon doping?*

Here we argue that composite pairing provides a natural resolution of this paradox. Due to its molecular nature, a composite d-wave superconductor has two components: a BCS component coexisting with a molecular superfluid. Both components contribute to the superfluid stiffness[7]. Upon doping (or through other external parameters), there can be a Lifshitz transition where the underlying heavy Fermi surface is depleted, transforming it into a Kondo insulator. As a result the BCS component of the superfluid vanishes, giving rise to a purely molecular superfluid of d-wave composite pairs (see Fig. 1(a)).

A d-wave condensate of composite pairs can be regarded as Bose-Einstein condensate of weakly interacting d-wave molecules in which the fermionic single particle excitation spectrum is fully gapped. The low energy excitations are governed by a linear sound mode with dispersion $v_s q$, which is cut off at low energies by the plasma frequency. For temperatures greater than the plasma frequency, the variation of the London penetration depth is governed by Landau's two-fluid picture of superfluidity, in which the excitation of the normal composite quasiparticles in two dimensions is predicted to give rise to a power law dependence of the penetration depth $\Delta\lambda(T) \sim T^3$, consistent with experiments[3].

A quantum critical point recently observed around $x \sim 0.2$ in transverse magnetore-

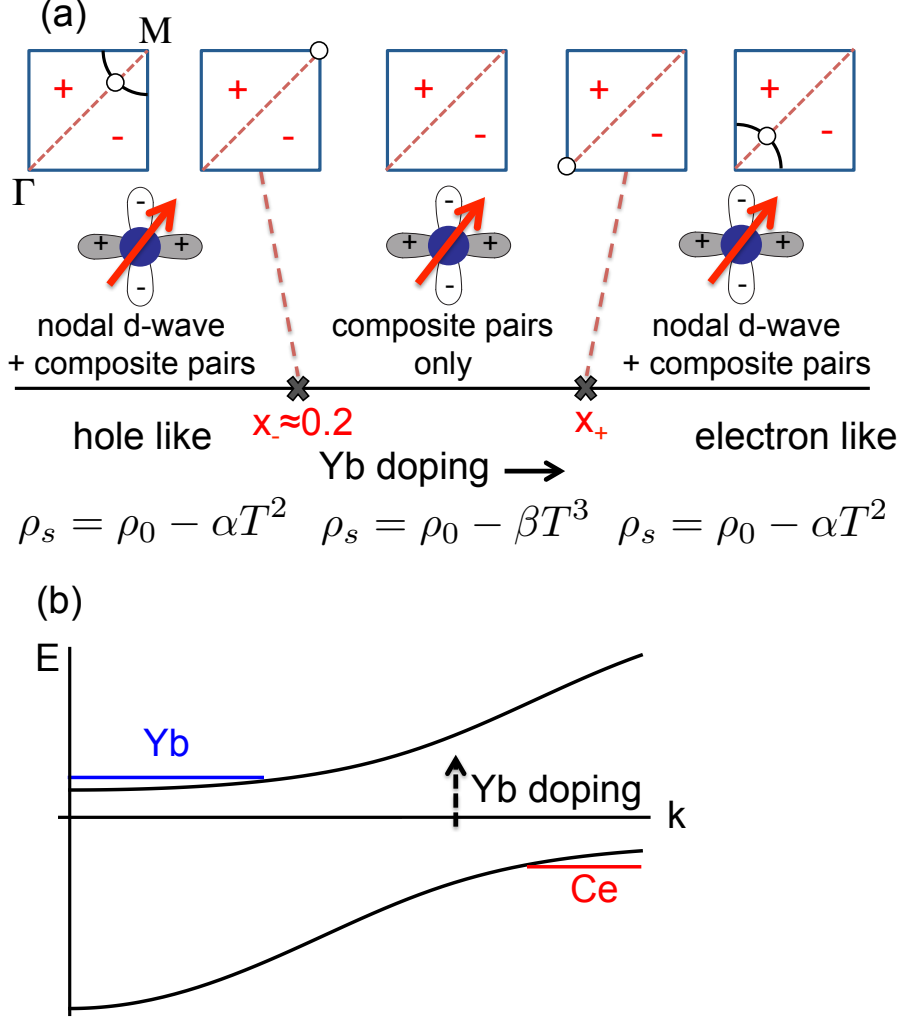


FIG. 1: (a) Schematic phase diagram for the $\text{Yb}_x\text{Ce}_{1-x}\text{CoIn}_5$. For $x < 0.2$ the temperature dependence of London penetration depth $\Delta\lambda \sim T - T^2$, consistent with nodal d-wave superconductivity in clean and dirty limits respectively. However for $x > 0.2$, the power law of the $\Delta\lambda$ exceeds 2 and reaches 3[3]. This is incompatible with nodal d-wave superconductivity and suggests a fully-gapped state. We argue that in the gapless phase Cooper pairs and composite pairs coexist whereas in the fully gapped phase, only the composite pairs are present. As function of Yb doping, chemical potential increases and the nodes of the order parameter moves to the corners of the Brillouin zone and annihilate. We predict that upon further doping, there is a second quantum phase transition to a reentrant gapless phase. (b) Schematic heavy fermion band structure. Ce Kondo lattice is hole-like whereas Yb Kondo lattice is electron-like. Thus upon Yb doping, chemical potential increases and heavy fermion band structure turns from hole-like to electron-like.

sistance measurements [8] can be related to the gapless to fully-gapped transition. Upon further Yb doping, we expect a second quantum critical point to a reentrant gapless phase as shown in Fig. 1(a) where the nodes reappear at the Γ point with the development of an underlying electron-like heavy Fermi surface in the underlying Yb rich Kondo lattice. We now expand on the idea of composite pairing and discuss its detailed application to Yb doped CeCoIn₅ and discuss the consequences and the predictions of our theory.

Composite pairing: The concept of composite pairing was first introduced in the context of odd-frequency pairing [9], and later associated with a different pairing mechanism in which a Cooper pair of conduction electrons binds to a local moment [7, 10–12]. Composite pairing naturally emerges within a two-channel Kondo model where the interference between two spin-screening channels give rise to local pairing. It can be thought of as an intra-orbital version of the resonating valence bond pairing [13, 14]. The amplitude of the composite pairing is

$$\Lambda_C(i) = \langle \psi_{1i}^\dagger \vec{\sigma}(i\sigma_2) \psi_{2i}^\dagger \cdot \vec{S}_f(i) \rangle \quad (1)$$

where $\psi_{1(2)}^\dagger$ creates conduction electrons in the Wannier state of channel 1(2) and $\vec{S}_f(i)$ describes the spin operator of the local f-moment at site i . The ψ 's can be represented by the plane waves as $\psi_{i\Gamma\sigma} = \sum_k \Phi_{\gamma k\sigma\sigma'} c_{k\sigma'} e^{i\mathbf{k}\cdot\mathbf{R}_i}$ where the form factor $\Phi_{\gamma k\sigma\sigma'}$ is only diagonal in the absence of spin-orbit coupling. Kondo couplings of the two channels, $J_{1(2)}$ can be derived by incorporating the virtual charge fluctuations from the ground state (singly occupied) to the excited states: empty and doubly occupied configurations.

The symmetry of the composite order $\Lambda_C(k)$ is determined by the product of the two form factors $\Phi_{1k}\Phi_{2k}$. For simplicity of discussion we shall choose Φ_{1k} and Φ_{2k} to be s-wave and nodal d-wave respectively, giving rise to a composite order parameter of nodal d-wave symmetry. The superfluid stiffness $Q = Q^{BCS} + Q^M$ of the condensate has two components[7], where

$$Q^{BCS} = \frac{ne^2}{m^*} \quad (2)$$

is the BCS contribution from the paired heavy electron fluid and

$$Q^M \simeq \sum_k \frac{\Lambda_C^2 (\Phi_{1k} \nabla \Phi_{2k} - \Phi_{2k} \nabla \Phi_{1k})^2}{\Sigma_N^2 \sqrt{\epsilon_k^2 + 2\Sigma_N^2}} \sim \frac{e^2}{\hbar a} (k_B T_c) \quad (3)$$

is the superfluid stiffness of the fluid of composite pairs. Here Σ_N is proportional to the normal (hybridization) part of the conduction electron self-energy and ϵ_k is the conduction

electron dispersion. In two dimensions, $Q^{BCS} \sim \epsilon_F/a$ is proportional to the Fermi energy. For conventional superconductors the superfluid stiffness is much greater than T_c . However, as the Fermi surface shrinks, Q^{BCS} vanishes. On the other hand the composite component of the superfluid stiffness Q^M , results from the mobility of the molecular pairs, derived ultimately from the non-local character (momentum dependence) of the Kondo form factors. Q_M is directly proportional to the condensation energy, a consequence of “local pair” condensation and it does not depend on the presence of a Fermi surface.

In the absence of a Fermi surface Q^{BCS} is zero and the only contribution to the superfluid stiffness derives from molecular pairing. For instance, consider a single channel Kondo model at half filling. The ground state is a Kondo insulator with a gap for quasiparticle excitations. The inclusion of a second Kondo channel leads to composite pairing beyond a critical ratio of the coupling constants[15]. As a result the fermionic single particle spectrum is fully-gapped even though the composite order parameter has nodal d-wave symmetry. This state is an example of a Bose-Einstein condensate of d-wave molecules.

Connection with Yb doped CeCoIn₅: The Kondo effect in both Ce and Yb heavy fermion compounds results from high frequency valence fluctuations. Ce heavy fermion compounds involve a predominant valence fluctuation between the $4f^1$ and $4f^0$ configuration $4f^1 \rightleftharpoons 4f^0 + e^-$, giving rise to an average f-occupation below unity, which by the Friedel sum rule gives rise to a scattering phase shift $\delta < \frac{\pi}{2}$ and hole-like heavy Fermi surfaces. By contrast, Yb heavy fermion materials involve valence fluctuations between the $4f^{13}$ and $4f^{14}$ configurations $e^- + 4f^{13} \rightleftharpoons 4f^{14}$, giving rise to an average f-occupation above unity, a scattering phase shift $\delta > \frac{\pi}{2}$ and an electron-like Fermi surface in the Kondo lattice (Fig. 1b). Upon Yb doping the phase shift of the resonant scattering increases and passes through $\pi/2$. At $\phi = \pi/2$, the Fermi surface collapses leading to a Kondo insulator immersed within a d-wave composite superfluid as described in the previous section. As a function of doping, the nodes of the gap move to the zone corner as shown in Fig. 1 (a) and annihilate. This predicted behavior should be observable in STM quasiparticle interference experiments.

Penetration depth: For nodal superconductors, the temperature dependence of the change of the penetration depth $\Delta\lambda(T) \sim T^n$ is either $n = 1$ in the clean limit or $n = 2$ in the dirty limit. A higher power is inconsistent with a nodal gap. Experiments[3] show that $n \sim 3$ for $x \sim 0.2$. The temperature dependence of the penetration depth of a fully-gapped molecular condensate is governed by the sound mode whose scale is set by the superfluid stiffness Q_C .

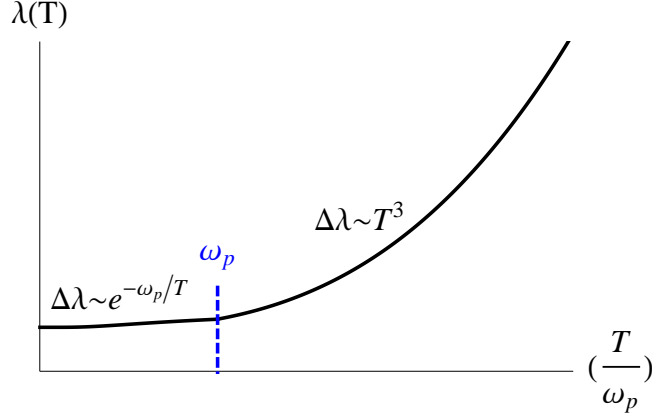


FIG. 2: Temperature dependence of the London penetration depth. For $T < \omega_p$, the $\Delta\lambda(T)$ is exponentially suppressed, whereas it crosses over to T^3 for $T > \omega_p$.

In a Landau two fluid model, the temperature dependence of the superfluid density is

$$\rho_s(T) = \rho_0 - \frac{(2e)^2}{d} \int \frac{d^d q}{(2\pi)^d} \left(-\frac{\partial n(\omega_q)}{\partial \epsilon_q} \right) v_s^2 \quad (4)$$

where d is the dimension. In two dimensions ρ_s is proportional to $\rho_s \propto \rho_0 - \alpha T^3$, which leads to the temperature dependence of the penetration depth to be $\lambda(T) = \lambda_0 + \beta T^3$ in agreement with experiments. The sound mode should be accessible to detect by the ultrasound experiments. Moreover since it is a charged condensate, the spectrum is gapped by the plasma frequency ω_p . We estimate the ω_p to be $10mK$. Thus the temperature dependence of the composite pairs has the power law $n = 3$ for $T > \omega_p$ as shown in Fig 2. This temperature dependence is consistent with experiments.

T_c as a function of doping: Another interesting consequence of the composite pairs is the doping dependence of T_c . Assuming composite pairs can only be created at Ce sites, the density of the bosons, n_B is directly proportional to the concentration of the Ce atoms $(1-x)$. In a two dimensional Bose-Einstein condensate, T_c is set by the density of bosons: $T_c \approx T_c(0) \times n_B$. Similarly in our case, $T_c \approx T_c(0) \times (1 - x)$.

Conclusion: Composite pairing provides a natural explanation for the fully-gapped state of Yb doped CeCoIn₅. As a function of Yb doping the chemical potential increases and the nodes move to the corner of the Brillouin zone. When the phase shift reaches $\pi/2$, the nodes annihilate, completely depleting the Fermi surface. Fully-gapped state has a superfluid stiffness coming from the molecular pairs. The sound mode as the low energy excitation of

the molecular condensate can be detected by ultrasound experiments. The unusual doping dependence of the T_c can be simply understood by BEC temperature of the composite pairs.

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